Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 02:37 AM EDT

PDB ID	:	4IFD
Title	:	Crystal structure of an 11-subunit eukaryotic exosome complex bound to RNA
Authors	:	Makino, D.L.; Conti, E.
Deposited on	:	2012-12-14
Resolution	:	2.81 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

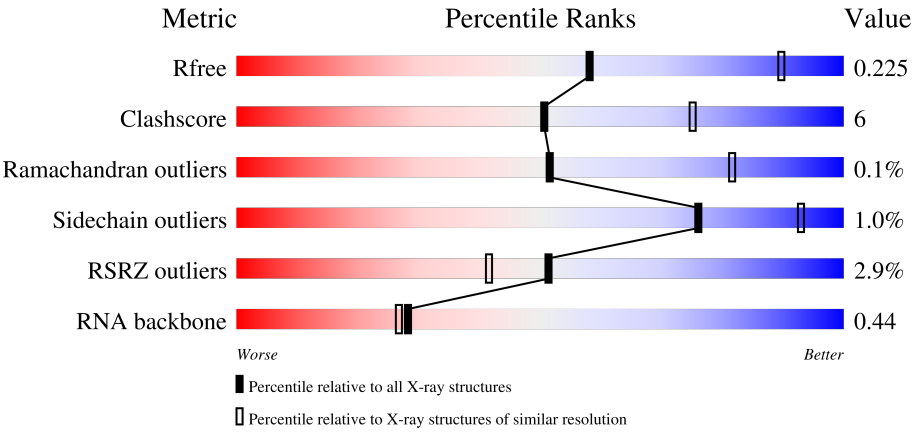
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	304	% 85% 13% ••
2	B	248	83% 14% •
3	C	393	3% 71% 15% 14%
4	D	245	79% 12% 9%

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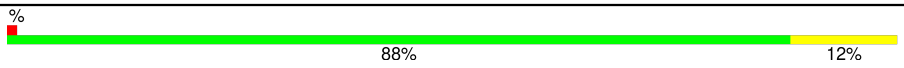
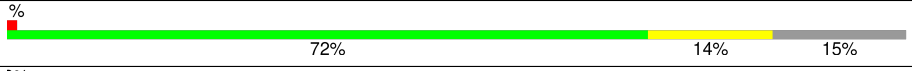
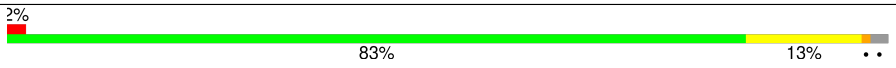
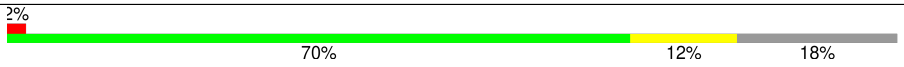
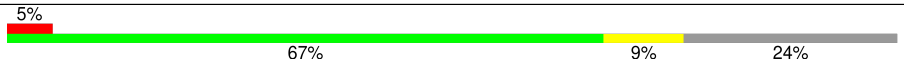
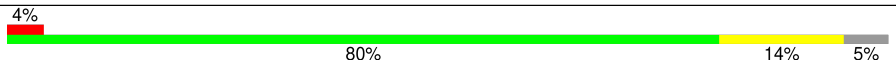
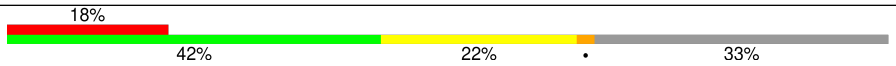
Mol	Chain	Length	Quality of chain
5	E	267	
6	F	250	
7	G	242	
8	H	361	
9	I	301	
10	J	1003	
11	K	179	
12	R	45	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	BR	A	402	-	-	X	-
13	BR	J	1101	-	-	X	-
13	BR	J	1102	-	-	X	-

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 26848 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Exosome complex component RRP45.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	300	2301	1443	394	448	16	0	0	0

- Molecule 2 is a protein called Exosome complex component SKI6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	242	1882	1177	336	361	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P46948
B	0	HIS	-	expression tag	UNP P46948

- Molecule 3 is a protein called Exosome complex component RRP43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	338	2627	1660	453	503	11	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	102	SER	ALA	engineered mutation	UNP P25359
C	363	MET	VAL	engineered mutation	UNP P25359

- Molecule 4 is a protein called Exosome complex component RRP46.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	223	1702	1070	288	334	10	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-21	GLY	-	expression tag	UNP P53256
D	-20	HIS	-	expression tag	UNP P53256
D	-19	GLY	-	expression tag	UNP P53256
D	-18	ASN	-	expression tag	UNP P53256
D	-17	ASN	-	expression tag	UNP P53256
D	-16	LYS	-	expression tag	UNP P53256
D	-15	GLU	-	expression tag	UNP P53256
D	-14	PRO	-	expression tag	UNP P53256
D	-13	ASN	-	expression tag	UNP P53256
D	-12	THR	-	expression tag	UNP P53256
D	-11	LYS	-	expression tag	UNP P53256
D	-10	ASN	-	expression tag	UNP P53256
D	-9	ARG	-	expression tag	UNP P53256
D	-8	LEU	-	expression tag	UNP P53256
D	-7	ASP	-	expression tag	UNP P53256
D	-6	SER	-	expression tag	UNP P53256
D	-5	ALA	-	expression tag	UNP P53256
D	-4	GLU	-	expression tag	UNP P53256
D	-3	LYS	-	expression tag	UNP P53256
D	-2	LYS	-	expression tag	UNP P53256
D	-1	LYS	-	expression tag	UNP P53256
D	0	LYS	-	expression tag	UNP P53256

- Molecule 5 is a protein called Exosome complex component RRP42.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	267	Total	C	N	O	S	0	0	0
			2042	1304	338	395	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	expression tag	UNP Q12277
E	0	HIS	-	expression tag	UNP Q12277
E	138	ILE	VAL	engineered mutation	UNP Q12277

- Molecule 6 is a protein called Exosome complex component MTR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	213	Total	C	N	O	S	0	0	0
			1640	1023	280	327	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	75	SER	THR	engineered mutation	UNP P48240
F	161	THR	MET	engineered mutation	UNP P48240

- Molecule 7 is a protein called Exosome complex component RRP40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	236	Total	C	N	O	S	0	0	0
			1804	1150	296	348	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP Q08285
G	0	HIS	-	expression tag	UNP Q08285

- Molecule 8 is a protein called Exosome complex component RRP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	295	Total	C	N	O	S	0	0	0
			2248	1400	405	431	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	ARG	-	expression tag	UNP P38792
H	0	SER	-	expression tag	UNP P38792

- Molecule 9 is a protein called Exosome complex component CSL4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	230	Total	C	N	O	S	0	0	0
			1711	1071	303	329	8			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-8	MET	-	expression tag	UNP P53859
I	-7	LYS	-	expression tag	UNP P53859
I	-6	HIS	-	expression tag	UNP P53859
I	-5	HIS	-	expression tag	UNP P53859

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-4	HIS	-	expression tag	UNP P53859
I	-3	HIS	-	expression tag	UNP P53859
I	-2	HIS	-	expression tag	UNP P53859
I	-1	HIS	-	expression tag	UNP P53859
I	0	PRO	-	expression tag	UNP P53859

- Molecule 10 is a protein called Exosome complex exonuclease DIS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	948	Total	C	N	O	S	0	0	0
			7430	4693	1310	1392	35			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-1	GLY	-	expression tag	UNP Q08162
J	0	ALA	-	expression tag	UNP Q08162
J	171	ASN	ASP	engineered mutation	UNP Q08162
J	551	ASN	ASP	engineered mutation	UNP Q08162

- Molecule 11 is a protein called Exosome complex exonuclease RRP6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	81	Total	C	N	O	S	0	0	0
			623	393	110	118	2			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	515	ARG	-	expression tag	UNP Q12149
K	516	SER	-	expression tag	UNP Q12149
K	517	MET	-	expression tag	UNP Q12149

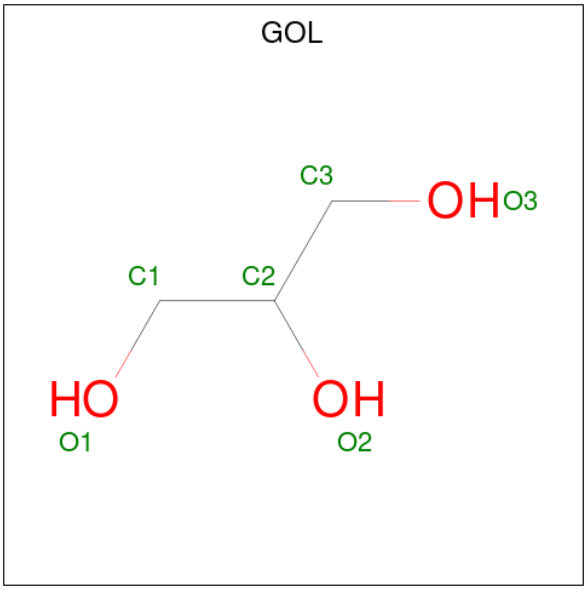
- Molecule 12 is a RNA chain called RNA (45-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	R	30	Total	C	N	O	P	0	0	0
			540	237	65	208	30			

- Molecule 13 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	2	Total Br 2 2	0	0
13	E	1	Total Br 1 1	0	0
13	F	1	Total Br 1 1	0	0
13	H	1	Total Br 1 1	0	0
13	I	1	Total Br 1 1	0	0
13	J	4	Total Br 4 4	0	0

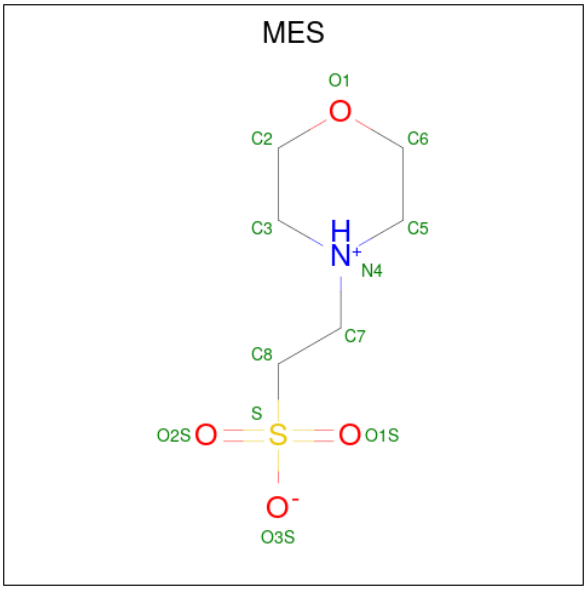
- Molecule 14 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	1	Total C O 6 3 3	0	0
14	G	1	Total C O 6 3 3	0	0
14	H	1	Total C O 6 3 3	0	0
14	H	1	Total C O 6 3 3	0	0
14	H	1	Total C O 6 3 3	0	0

- Molecule 15 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES)

(formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	J	1	Total	Mg	0	0
			1	1		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	J	1	Total	Zn	0	0
			1	1		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	35	Total	O	0	0
			35	35		
18	B	35	Total	O	0	0
			35	35		
18	C	20	Total	O	0	0
			20	20		
18	D	38	Total	O	0	0
			38	38		

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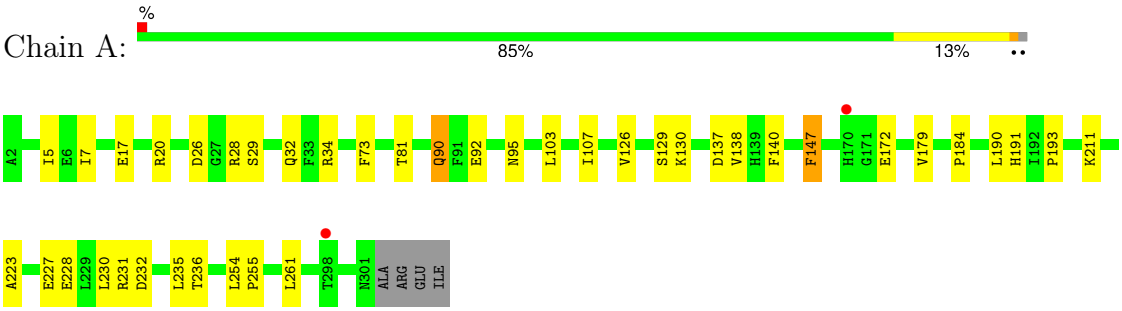
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	E	23	Total O 23 23	0	0
18	F	15	Total O 15 15	0	0
18	G	19	Total O 19 19	0	0
18	H	23	Total O 23 23	0	0
18	I	6	Total O 6 6	0	0
18	J	27	Total O 27 27	0	0
18	K	2	Total O 2 2	0	0
18	R	1	Total O 1 1	0	0

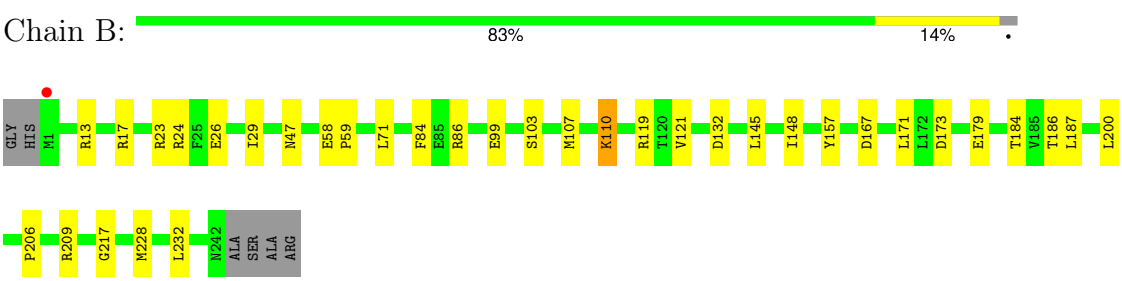
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

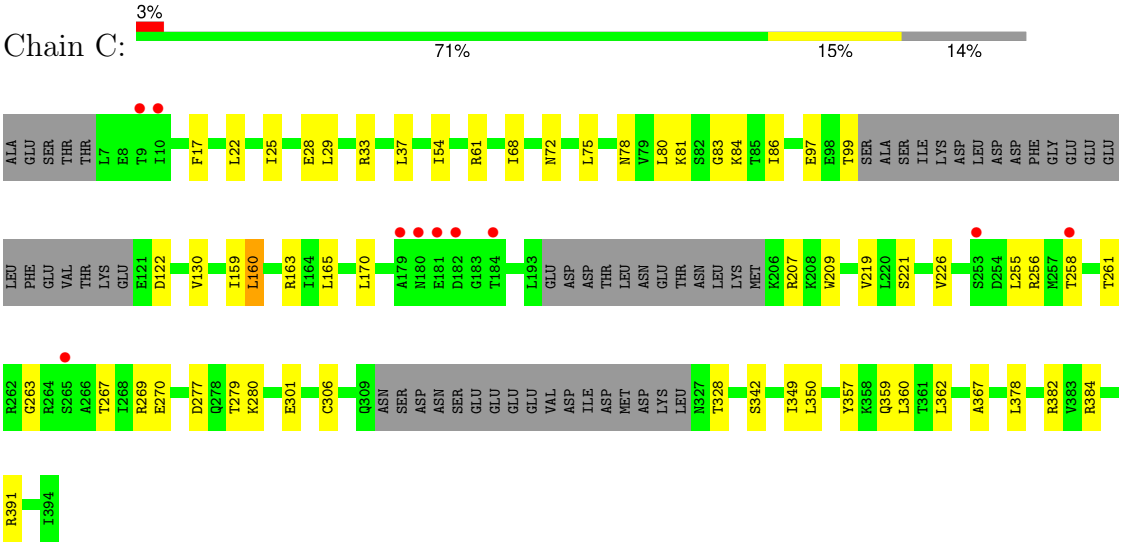
• Molecule 1: Exosome complex component RRP45



• Molecule 2: Exosome complex component SKI6

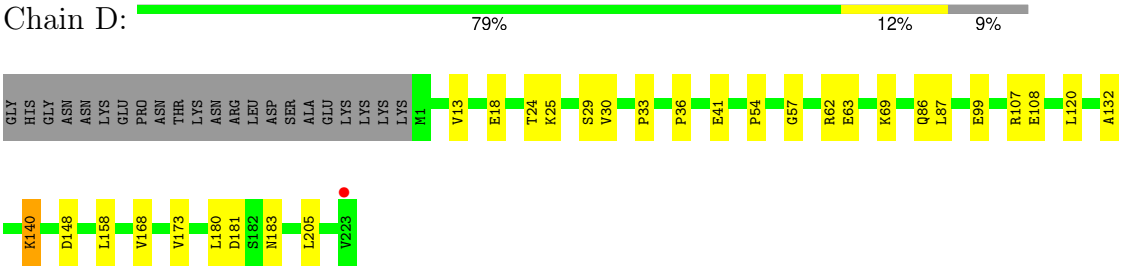


• Molecule 3: Exosome complex component RRP43



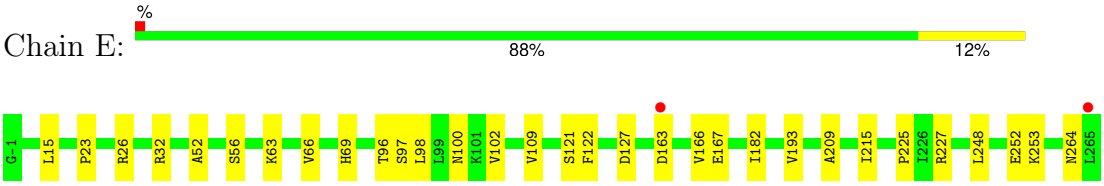
• Molecule 4: Exosome complex component RRP46

Chain D:



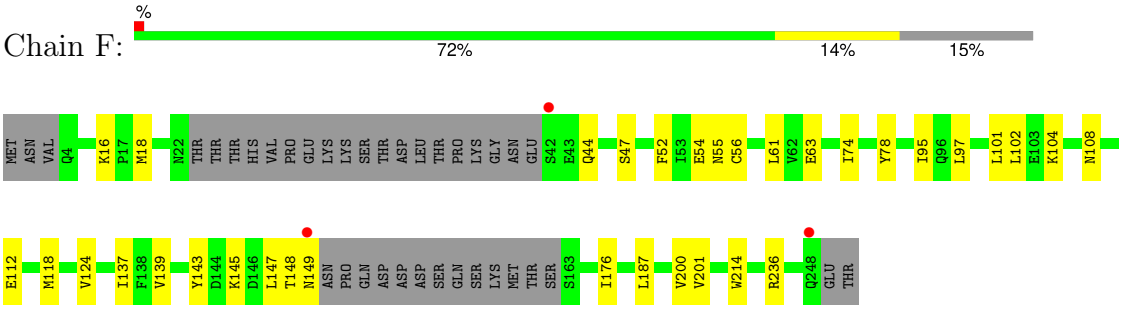
• Molecule 5: Exosome complex component RRP42

Chain E:



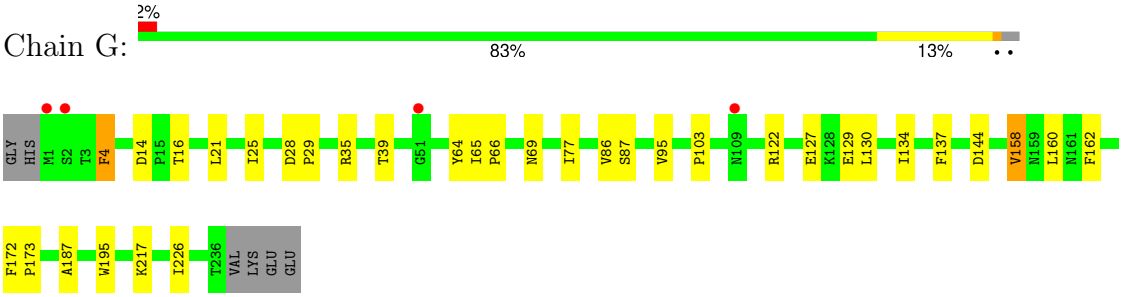
• Molecule 6: Exosome complex component MTR3

Chain F:



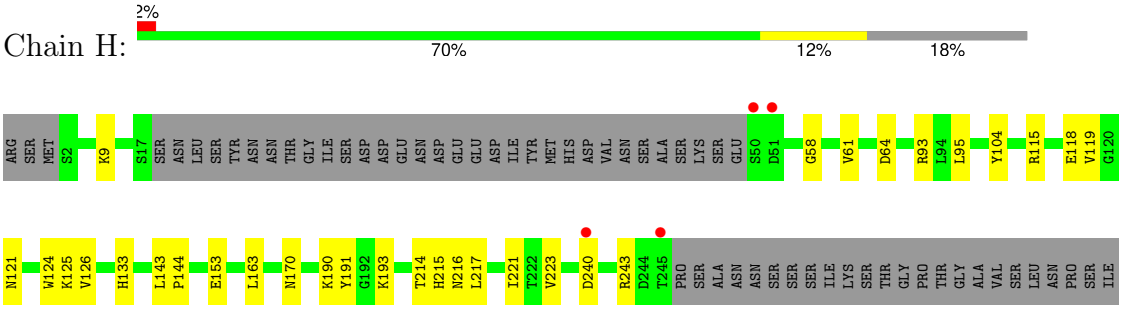
• Molecule 7: Exosome complex component RRP40

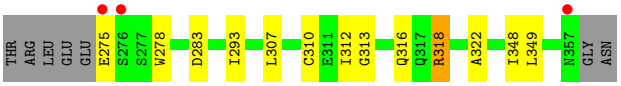
Chain G:



• Molecule 8: Exosome complex component RRP4

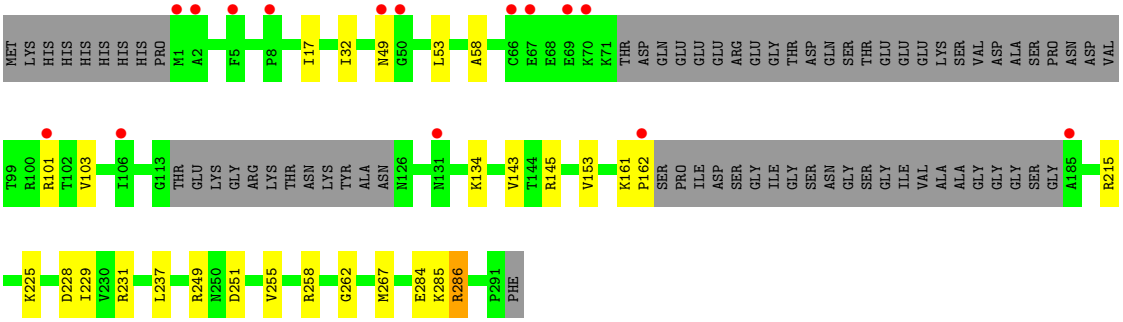
Chain H:





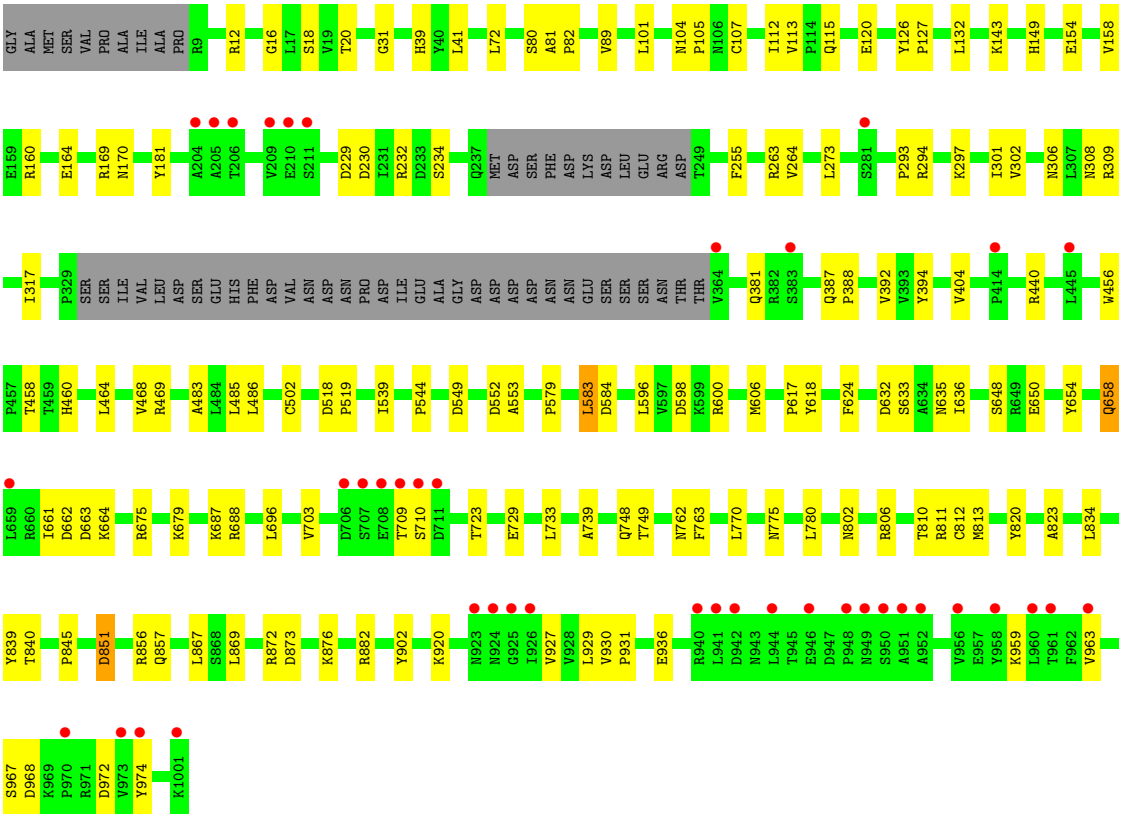
• Molecule 9: Exosome complex component CSL4

Chain I:



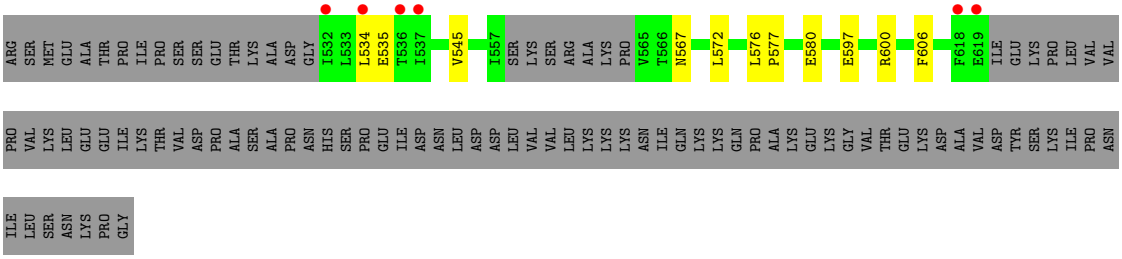
• Molecule 10: Exosome complex exonuclease DIS3

Chain J:



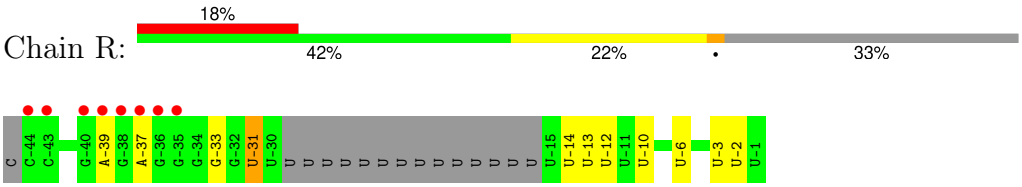
• Molecule 11: Exosome complex exonuclease RRP6

Chain K:



• Molecule 12: RNA (45-MER)

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	154.09Å 107.44Å 150.46Å 90.00° 110.63° 90.00°	Depositor
Resolution (Å)	49.64 – 2.81 49.64 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.9 (49.64-2.81) 87.9 (49.64-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.182 , 0.224 0.186 , 0.225	Depositor DCC
R_{free} test set	4956 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	54.9	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.020 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26848	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BR, ZN, GOL, MES, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.21	0/2337	0.35	0/3158
2	B	0.20	0/1906	0.36	0/2570
3	C	0.20	0/2670	0.38	0/3619
4	D	0.20	0/1720	0.39	0/2335
5	E	0.21	0/2082	0.37	0/2834
6	F	0.21	0/1662	0.37	0/2240
7	G	0.21	0/1841	0.37	0/2503
8	H	0.21	0/2282	0.38	0/3086
9	I	0.20	0/1735	0.38	0/2354
10	J	0.20	0/7575	0.37	0/10290
11	K	0.21	0/629	0.37	0/850
12	R	0.15	0/595	0.75	0/919
All	All	0.20	0/27034	0.39	0/36758

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2301	0	2262	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1882	0	1917	22	0
3	C	2627	0	2668	44	0
4	D	1702	0	1755	20	0
5	E	2042	0	2057	23	0
6	F	1640	0	1610	27	0
7	G	1804	0	1763	18	0
8	H	2248	0	2207	27	0
9	I	1711	0	1676	21	0
10	J	7430	0	7347	93	0
11	K	623	0	626	11	0
12	R	540	0	273	3	0
13	A	2	0	0	3	0
13	E	1	0	0	0	0
13	F	1	0	0	0	0
13	H	1	0	0	0	0
13	I	1	0	0	0	0
13	J	4	0	0	10	0
14	C	6	0	8	0	0
14	G	6	0	8	0	0
14	H	18	0	24	2	0
15	G	12	0	12	1	0
16	J	1	0	0	0	0
17	J	1	0	0	0	0
18	A	35	0	0	0	0
18	B	35	0	0	0	0
18	C	20	0	0	0	0
18	D	38	0	0	1	0
18	E	23	0	0	1	0
18	F	15	0	0	1	0
18	G	19	0	0	0	0
18	H	23	0	0	0	0
18	I	6	0	0	1	0
18	J	27	0	0	0	0
18	K	2	0	0	0	0
18	R	1	0	0	0	0
All	All	26848	0	26213	300	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (300) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:606:MET:HG2	13:J:1102:BR:BR	2.24	0.93
1:A:73:PHE:HB2	13:A:402:BR:BR	2.30	0.87
10:J:293:PRO:HG2	13:J:1101:BR:BR	2.41	0.75
6:F:44:GLN:HB3	6:F:236:ARG:HH12	1.51	0.74
8:H:143:LEU:HB3	8:H:144:PRO:HD2	1.71	0.73
1:A:172:GLU:HG2	3:C:269:ARG:HD2	1.70	0.73
4:D:33:PRO:HB2	4:D:86:GLN:HG2	1.70	0.72
6:F:44:GLN:HB3	6:F:236:ARG:NH1	2.05	0.72
10:J:811:ARG:NH2	10:J:936:GLU:OE2	2.22	0.71
3:C:357:TYR:OH	3:C:382:ARG:NH1	2.23	0.71
8:H:216:ASN:HD21	8:H:240:ASP:HB3	1.54	0.71
3:C:362:LEU:HB2	4:D:180:LEU:HB3	1.73	0.71
8:H:313:GLY:O	8:H:318:ARG:NH1	2.25	0.69
2:B:148:ILE:HG21	2:B:232:LEU:HD21	1.73	0.69
9:I:249:ARG:NH1	9:I:251:ASP:OD1	2.27	0.68
10:J:18:SER:HB2	10:J:41:LEU:HB2	1.74	0.68
10:J:688:ARG:NH1	10:J:729:GLU:OE2	2.27	0.67
10:J:294:ARG:HG3	13:J:1101:BR:BR	2.51	0.66
10:J:633:SER:HB3	10:J:635:ASN:HD21	1.60	0.66
11:K:597:GLU:HG3	11:K:600:ARG:HH11	1.61	0.66
10:J:549:ASP:OD1	10:J:600:ARG:NH1	2.29	0.66
8:H:214:THR:O	8:H:243:ARG:NH2	2.29	0.66
10:J:115:GLN:HB2	10:J:149:HIS:HA	1.77	0.65
5:E:26:ARG:NH1	5:E:32:ARG:HG3	2.11	0.64
10:J:661:ILE:HG23	10:J:675:ARG:HG2	1.80	0.64
4:D:36:PRO:HB3	4:D:87:LEU:HB2	1.80	0.63
4:D:13:VAL:HG11	4:D:29:SER:HB2	1.80	0.63
5:E:264:ASN:HB2	8:H:9:LYS:HE3	1.80	0.63
10:J:762:ASN:HB3	10:J:812:CYS:HB2	1.81	0.63
9:I:103:VAL:HG11	11:K:534:LEU:HD21	1.80	0.63
10:J:658:GLN:NE2	10:J:662:ASP:OD2	2.31	0.63
10:J:107:CYS:O	10:J:143:LYS:NZ	2.32	0.63
10:J:696:LEU:HD23	10:J:810:THR:HG23	1.79	0.63
1:A:137:ASP:OD2	4:D:57:GLY:N	2.28	0.63
5:E:109:VAL:HG13	5:E:182:ILE:HD11	1.80	0.63
2:B:179:GLU:HG2	2:B:184:THR:HG21	1.82	0.62
10:J:633:SER:HB3	10:J:635:ASN:ND2	2.15	0.62
10:J:606:MET:CG	13:J:1102:BR:BR	3.01	0.61
3:C:258:THR:HG22	3:C:267:THR:HG22	1.83	0.60
10:J:658:GLN:HG2	10:J:723:THR:HG23	1.84	0.60
10:J:81:ALA:HB1	10:J:82:PRO:HA	1.83	0.60
3:C:122:ASP:O	3:C:163:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:217:LYS:HD2	7:G:226:ILE:HD11	1.84	0.58
2:B:119:ARG:NH1	12:R:-31:U:H2'	2.17	0.58
6:F:97:LEU:HD22	6:F:139:VAL:HB	1.86	0.58
1:A:26:ASP:OD2	1:A:28:ARG:NE	2.29	0.58
6:F:200:VAL:HB	6:F:214:TRP:HB3	1.86	0.57
10:J:617:PRO:HA	10:J:648:SER:HB3	1.85	0.57
9:I:145:ARG:NH2	18:I:405:HOH:O	2.36	0.57
1:A:179:VAL:HG23	1:A:184:PRO:HD3	1.86	0.57
2:B:17:ARG:NH1	2:B:23:ARG:HG3	2.20	0.56
8:H:193:LYS:NZ	8:H:283:ASP:OD1	2.22	0.56
3:C:349:ILE:HG12	3:C:360:LEU:HD23	1.88	0.56
1:A:211:LYS:NZ	8:H:58:GLY:O	2.36	0.56
3:C:207:ARG:NH1	3:C:270:GLU:O	2.39	0.55
10:J:308:ASN:HB3	10:J:392:VAL:HG22	1.88	0.55
5:E:166:VAL:HG23	10:J:263:ARG:NH1	2.21	0.55
3:C:86:ILE:HD13	11:K:576:LEU:HD22	1.87	0.55
3:C:359[A]:GLN:NE2	4:D:183:ASN:OD1	2.39	0.55
3:C:160:LEU:O	3:C:160:LEU:HD12	2.07	0.55
7:G:69:ASN:OD1	7:G:122:ARG:NH1	2.39	0.55
4:D:86:GLN:NE2	18:D:305:HOH:O	2.39	0.55
10:J:636:ILE:HD11	10:J:733:LEU:HD11	1.87	0.55
2:B:84:PHE:O	5:E:63:LYS:NZ	2.37	0.55
8:H:118:GLU:OE2	8:H:125:LYS:HD2	2.07	0.55
1:A:5:ILE:HD11	1:A:90:GLN:HG2	1.87	0.54
6:F:61:LEU:HD23	6:F:74:ILE:HG12	1.89	0.54
10:J:12:ARG:NH1	10:J:154:GLU:OE2	2.40	0.54
10:J:539:ILE:HG22	10:J:648:SER:HA	1.89	0.54
3:C:75:LEU:HD11	6:F:18:MET:HE1	1.90	0.54
10:J:539:ILE:HG23	10:J:553:ALA:HB1	1.89	0.54
5:E:96:THR:O	5:E:100:ASN:ND2	2.36	0.54
1:A:7:ILE:HG21	1:A:230:LEU:HD21	1.90	0.54
8:H:322:ALA:HB2	8:H:348:ILE:HD11	1.90	0.54
3:C:165[B]:LEU:HD21	3:C:170:LEU:HD11	1.89	0.53
2:B:13:ARG:HD3	2:B:171:LEU:HD22	1.89	0.53
5:E:97:SER:HB2	6:F:108:ASN:HB3	1.90	0.53
10:J:120:GLU:OE2	10:J:170:ASN:ND2	2.31	0.53
3:C:75:LEU:HD21	6:F:18:MET:HE1	1.90	0.53
4:D:107:ARG:NH2	4:D:148:ASP:OD1	2.41	0.53
10:J:160:ARG:NH1	10:J:164:GLU:O	2.41	0.53
10:J:632:ASP:OD1	10:J:679:LYS:NZ	2.41	0.53
6:F:236:ARG:NH2	18:F:411:HOH:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:293:PRO:HD2	13:J:1101:BR:BR	2.64	0.53
9:I:143:VAL:HA	9:I:153:VAL:HG12	1.91	0.53
6:F:147:LEU:C	6:F:149:ASN:H	2.12	0.52
1:A:130:LYS:HE3	3:C:99:THR:HG21	1.91	0.52
3:C:84:LYS:HE3	6:F:54:GLU:HG3	1.92	0.52
3:C:349:ILE:HD13	3:C:378:LEU:HD23	1.90	0.52
5:E:15:LEU:HD11	5:E:23:PRO:HD3	1.90	0.52
10:J:297:LYS:O	10:J:381:GLN:NE2	2.43	0.52
6:F:148:THR:O	6:F:149:ASN:C	2.48	0.52
4:D:140:LYS:HA	4:D:158:LEU:HG	1.91	0.52
6:F:137:ILE:HG21	6:F:176:ILE:HG23	1.92	0.52
10:J:749:THR:O	10:J:857:GLN:NE2	2.43	0.52
10:J:485:LEU:HD21	10:J:596:LEU:HD11	1.92	0.51
10:J:839:TYR:OH	12:R:-3:U:OP1	2.27	0.51
10:J:264:VAL:HA	10:J:273:LEU:HD12	1.92	0.51
3:C:81:LYS:NZ	11:K:576:LEU:O	2.28	0.51
7:G:28:ASP:OD2	7:G:35:ARG:NH1	2.43	0.51
7:G:95:VAL:HG11	7:G:134:ILE:HG23	1.91	0.51
3:C:22:LEU:HD11	3:C:29:LEU:HD23	1.93	0.51
10:J:618:TYR:OH	10:J:650:GLU:OE1	2.22	0.51
7:G:77:ILE:HD13	7:G:87:SER:HB2	1.93	0.51
2:B:59:PRO:HG3	2:B:121:VAL:HG23	1.93	0.51
3:C:350:LEU:HB2	3:C:359[A]:GLN:HB3	1.92	0.51
3:C:362:LEU:HD22	4:D:180:LEU:HD23	1.93	0.51
8:H:124:TRP:NE1	8:H:163:LEU:O	2.44	0.50
3:C:61:ARG:HB3	3:C:72:ASN:HB3	1.91	0.50
3:C:68:ILE:HD12	3:C:279:THR:HG23	1.92	0.50
7:G:103:PRO:HG3	7:G:144:ASP:HB3	1.93	0.50
3:C:219:VAL:HG11	3:C:226:VAL:HG21	1.93	0.50
2:B:29:ILE:HD11	2:B:145:LEU:HD22	1.93	0.50
7:G:21:LEU:HD22	7:G:25:ILE:HG21	1.94	0.50
2:B:187:LEU:HD12	2:B:217:GLY:HA3	1.94	0.50
5:E:166:VAL:HG23	10:J:263:ARG:HH11	1.76	0.50
10:J:544:PRO:HD3	10:J:654:TYR:HE2	1.78	0.49
5:E:69:HIS:ND1	5:E:121:SER:OG	2.40	0.49
3:C:301:GLU:HG2	3:C:328:THR:HG22	1.93	0.49
2:B:24:ARG:HH11	2:B:26:GLU:CD	2.15	0.49
8:H:307:LEU:HD21	8:H:348:ILE:HD12	1.95	0.49
6:F:56:CYS:HB3	6:F:78:TYR:CZ	2.48	0.49
8:H:153:GLU:OE2	9:I:215:ARG:NH2	2.39	0.49
3:C:83:GLY:HA2	11:K:580:GLU:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:148:THR:O	6:F:149:ASN:O	2.30	0.48
10:J:158:VAL:O	10:J:169:ARG:NH1	2.46	0.48
1:A:103:LEU:O	1:A:107:ILE:HG12	2.12	0.48
4:D:132:ALA:HB1	4:D:205:LEU:HD23	1.94	0.48
7:G:187:ALA:HB3	7:G:195:TRP:HB3	1.93	0.48
10:J:663:ASP:OD1	10:J:664:LYS:N	2.46	0.48
7:G:14:ASP:OD2	7:G:16:THR:OG1	2.31	0.48
7:G:127:GLU:HB2	7:G:130:LEU:HB3	1.94	0.48
8:H:310:CYS:HB2	8:H:312:ILE:HG12	1.96	0.48
9:I:225:LYS:HG3	9:I:286:ARG:NH1	2.28	0.48
7:G:129:GLU:OE2	9:I:225:LYS:HE3	2.14	0.48
1:A:92:GLU:HB2	1:A:95:ASN:HB2	1.95	0.48
8:H:217:LEU:HD11	8:H:223:VAL:HG12	1.96	0.47
3:C:37:LEU:HD12	11:K:606:PHE:HD1	1.79	0.47
10:J:101:LEU:HD13	10:J:234:SER:HB2	1.95	0.47
1:A:126:VAL:HG23	1:A:130:LYS:H	1.80	0.47
3:C:280:LYS:NZ	3:C:280:LYS:HB3	2.30	0.47
6:F:16:LYS:NZ	6:F:16:LYS:HB3	2.30	0.47
10:J:293:PRO:CG	13:J:1101:BR:BR	3.17	0.47
1:A:191:HIS:CE1	1:A:193:PRO:HG3	2.50	0.47
8:H:118:GLU:HG2	8:H:125:LYS:HB2	1.97	0.47
9:I:228:ASP:OD2	9:I:286:ARG:NE	2.48	0.47
10:J:20:THR:HG23	10:J:39:HIS:HB3	1.96	0.47
10:J:294:ARG:HB2	13:J:1101:BR:BR	2.69	0.47
10:J:802:ASN:OD1	10:J:806:ARG:NH2	2.47	0.47
9:I:161:LYS:O	9:I:162:PRO:C	2.52	0.47
10:J:460:HIS:CD2	10:J:464:LEU:HD11	2.50	0.47
1:A:126:VAL:HG23	1:A:129:SER:HB2	1.97	0.47
3:C:28:GLU:OE2	3:C:342:SER:HB2	2.14	0.47
3:C:17:PHE:HZ	9:I:255:VAL:HG11	1.80	0.46
5:E:163:ASP:HA	5:E:167:GLU:HA	1.97	0.46
10:J:920:LYS:HB3	10:J:927:VAL:HB	1.97	0.46
4:D:36:PRO:HG2	4:D:41:GLU:HG2	1.96	0.46
10:J:869:LEU:HD23	10:J:872:ARG:NH1	2.29	0.46
10:J:12:ARG:NH2	10:J:16:GLY:O	2.48	0.46
10:J:229:ASP:HA	10:J:232:ARG:HE	1.80	0.46
10:J:294:ARG:CG	13:J:1101:BR:BR	3.18	0.46
10:J:404:VAL:HG11	10:J:483:ALA:HB1	1.97	0.46
9:I:231:ARG:NH1	9:I:251:ASP:O	2.45	0.46
10:J:104:ASN:O	10:J:143:LYS:NZ	2.33	0.46
2:B:13:ARG:NH1	2:B:171:LEU:HB3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:86:VAL:HG11	7:G:134:ILE:HD11	1.97	0.46
10:J:302:VAL:O	10:J:306:ASN:ND2	2.43	0.46
5:E:215:ILE:HD13	5:E:248:LEU:HD23	1.98	0.46
10:J:770:LEU:O	10:J:775:ASN:N	2.49	0.46
9:I:101:ARG:NH1	11:K:535:GLU:HA	2.30	0.45
9:I:134:LYS:HD2	9:I:237:LEU:HD21	1.97	0.45
8:H:115:ARG:HE	14:H:403:GOL:H31	1.82	0.45
4:D:69:LYS:NZ	4:D:181:ASP:OD2	2.42	0.45
1:A:190:LEU:HD23	10:J:748:GLN:HG3	1.98	0.45
3:C:54:ILE:HB	3:C:78:ASN:HD21	1.81	0.45
5:E:98:LEU:O	5:E:102:VAL:HG23	2.16	0.45
2:B:17:ARG:HH12	2:B:173:ASP:HB3	1.82	0.45
6:F:52:PHE:CE2	6:F:61:LEU:HB2	2.52	0.45
10:J:739:ALA:HB2	10:J:840:THR:HG22	1.98	0.45
5:E:66:VAL:HG21	10:J:31:GLY:HA2	1.99	0.45
3:C:207:ARG:HE	3:C:269:ARG:HH21	1.65	0.45
6:F:47:SER:HA	11:K:567:ASN:HB2	1.98	0.45
10:J:820:TYR:CZ	10:J:823:ALA:HB2	2.51	0.45
1:A:73:PHE:CB	13:A:402:BR:BR	3.14	0.45
1:A:172:GLU:OE2	3:C:256:ARG:NH2	2.50	0.45
10:J:867:LEU:O	10:J:872:ARG:NH1	2.45	0.45
10:J:929:LEU:HD13	10:J:936:GLU:HG2	1.99	0.45
2:B:71:LEU:HB2	2:B:121:VAL:HG22	1.97	0.44
5:E:52:ALA:HB3	5:E:56:SER:HB2	1.99	0.44
5:E:193:VAL:HG22	5:E:209:ALA:HA	1.99	0.44
2:B:86:ARG:NH1	5:E:127:ASP:OD1	2.51	0.44
5:E:252:GLU:OE2	18:E:418:HOH:O	2.21	0.44
6:F:124:VAL:HG12	6:F:187:LEU:HD22	1.99	0.44
6:F:47:SER:HB3	6:F:63:GLU:HB2	1.99	0.44
7:G:172:PHE:HA	7:G:173:PRO:HD3	1.79	0.44
8:H:312:ILE:HD12	8:H:349:LEU:HD21	1.99	0.44
8:H:190:LYS:HE3	8:H:191:TYR:CZ	2.53	0.44
4:D:99:GLU:OE2	4:D:108:GLU:HG3	2.17	0.44
6:F:143:TYR:HE2	6:F:145:LYS:HE2	1.82	0.44
3:C:263:GLY:HA3	10:J:882:ARG:NH1	2.32	0.43
3:C:97:GLU:HG2	3:C:209:TRP:CD1	2.52	0.43
10:J:309:ARG:NH1	10:J:458:THR:HG22	2.33	0.43
3:C:33:ARG:NH1	3:C:306:CYS:HA	2.34	0.43
3:C:301:GLU:HG3	3:C:367:ALA:HB2	2.01	0.43
9:I:258:ARG:HB2	9:I:262:GLY:HA2	2.00	0.43
1:A:17:GLU:OE2	1:A:20:ARG:NE	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:HD23	2:B:99:GLU:HG3	2.00	0.43
10:J:468:VAL:HG12	10:J:469:ARG:HG3	2.00	0.43
2:B:206:PRO:HB2	2:B:209:ARG:HD3	1.98	0.43
8:H:221:ILE:HG22	8:H:293:ILE:HG23	2.00	0.43
10:J:317:ILE:HB	10:J:394:TYR:HB3	2.01	0.43
10:J:959:LYS:HD3	10:J:972:ASP:OD2	2.19	0.43
4:D:62:ARG:NH2	4:D:108:GLU:OE2	2.50	0.43
8:H:104:TYR:HD1	14:H:402:GOL:H2	1.82	0.43
10:J:387:GLN:HA	10:J:388:PRO:HD3	1.80	0.43
5:E:227:ARG:NH1	6:F:112:GLU:OE2	2.51	0.43
10:J:873:ASP:HB3	10:J:876:LYS:HB2	2.00	0.43
8:H:124:TRP:CE2	8:H:163:LEU:HB2	2.54	0.43
10:J:959:LYS:HE2	10:J:974:TYR:HE1	1.84	0.43
5:E:15:LEU:HD23	5:E:193:VAL:HG21	2.00	0.43
7:G:64:TYR:HA	7:G:160:LEU:HD11	2.01	0.43
8:H:215:HIS:ND1	8:H:316:GLN:HB3	2.33	0.43
10:J:230:ASP:OD1	10:J:440:ARG:NH2	2.52	0.43
10:J:579:PRO:HA	10:J:584:ASP:OD2	2.19	0.43
1:A:235:LEU:HD22	1:A:261:LEU:HD22	2.01	0.42
1:A:254:LEU:HD12	1:A:255:PRO:HD2	2.01	0.42
2:B:58:GLU:HG3	8:H:133:HIS:CG	2.55	0.42
5:E:102:VAL:HG22	5:E:225:PRO:HD2	2.01	0.42
12:R:-3:U:H2'	12:R:-2:U:C6	2.54	0.42
3:C:130:VAL:HG22	3:C:159:ILE:HD12	2.01	0.42
5:E:227:ARG:HD2	6:F:214:TRP:CE3	2.54	0.42
8:H:170:ASN:HB2	8:H:191:TYR:HA	2.00	0.42
10:J:579:PRO:HG3	10:J:856:ARG:NH1	2.34	0.42
3:C:72:ASN:HA	6:F:102:LEU:HD11	2.00	0.42
9:I:267:MET:HE1	9:I:284:GLU:OE1	2.20	0.42
10:J:709:THR:OG1	10:J:710:SER:N	2.53	0.42
10:J:104:ASN:HA	10:J:105:PRO:HD3	1.87	0.42
10:J:502:CYS:HB2	10:J:583:LEU:HD12	2.01	0.42
3:C:25:ILE:HG23	9:I:229:ILE:HG13	2.02	0.42
4:D:18:GLU:OE2	4:D:25:LYS:HD2	2.19	0.42
15:G:302:MES:H51	15:G:302:MES:H81	1.77	0.42
8:H:275:GLU:HA	8:H:278:TRP:HD1	1.85	0.42
3:C:277:ASP:OD1	3:C:280:LYS:N	2.45	0.42
10:J:967:SER:OG	10:J:968:ASP:N	2.53	0.42
2:B:186:THR:HB	2:B:200:LEU:HB3	2.02	0.42
10:J:126:TYR:N	10:J:127:PRO:HD2	2.35	0.42
10:J:635:ASN:OD1	10:J:687:LYS:NZ	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLU:HG3	1:A:231:ARG:CZ	2.49	0.41
10:J:703:VAL:HG11	10:J:902:TYR:HB3	2.02	0.41
10:J:930:VAL:HA	10:J:931:PRO:HD2	1.96	0.41
1:A:28:ARG:CZ	1:A:34:ARG:HG3	2.51	0.41
1:A:73:PHE:N	13:A:402:BR:BR	3.01	0.41
1:A:223:ALA:HB1	1:A:227:GLU:HB2	2.02	0.41
8:H:64:ASP:OD2	8:H:93:ARG:NH1	2.52	0.41
10:J:618:TYR:HA	13:J:1104:BR:BR	2.75	0.41
10:J:518:ASP:HA	10:J:519:PRO:HD3	1.93	0.41
11:K:572:LEU:HB3	11:K:576:LEU:HG	2.01	0.41
1:A:29:SER:HB3	1:A:32:GLN:HB2	2.02	0.41
1:A:81:THR:HG22	1:A:138:VAL:HB	2.02	0.41
1:A:232:ASP:O	2:B:110:LYS:NZ	2.54	0.41
9:I:32:ILE:HB	9:I:103:VAL:HG22	2.03	0.41
1:A:107:ILE:HG21	1:A:236:THR:HG21	2.02	0.41
2:B:103:SER:O	2:B:107:MET:HG3	2.21	0.41
7:G:158:VAL:HG13	7:G:162:PHE:HB3	2.01	0.41
10:J:255:PHE:CB	10:J:309:ARG:HH11	2.33	0.41
2:B:157:TYR:HD2	2:B:228:MET:HE2	1.86	0.41
3:C:221:SER:HA	6:F:55:ASN:HB2	2.02	0.41
5:E:253:LYS:HE3	5:E:253:LYS:HB2	1.91	0.41
9:I:32:ILE:HG13	9:I:101:ARG:HE	1.86	0.41
10:J:309:ARG:HD2	10:J:456:TRP:CD1	2.56	0.41
4:D:24:THR:OG1	4:D:107:ARG:NH1	2.54	0.41
8:H:61:VAL:HG11	8:H:95:LEU:HD21	2.02	0.41
10:J:763:PHE:CG	10:J:780:LEU:HD21	2.55	0.41
2:B:47:ASN:OD1	2:B:132:ASP:N	2.52	0.41
7:G:4:PHE:HE2	7:G:39:THR:HG22	1.86	0.41
9:I:285:LYS:C	9:I:286:ARG:HG2	2.41	0.41
10:J:81:ALA:CB	10:J:82:PRO:HA	2.45	0.41
10:J:301:ILE:HD13	10:J:392:VAL:HG12	2.03	0.41
10:J:851:ASP:OD1	10:J:851:ASP:N	2.53	0.41
3:C:33:ARG:HH12	3:C:306:CYS:HA	1.85	0.41
9:I:53:LEU:HD11	11:K:545:VAL:HG13	2.01	0.41
10:J:845:PRO:HA	10:J:851:ASP:HB2	2.03	0.41
10:J:959:LYS:HE2	10:J:974:TYR:CE1	2.56	0.41
3:C:350:LEU:HB2	3:C:359[B]:GLN:HB3	2.04	0.40
6:F:95:ILE:H	6:F:118:MET:HE3	1.86	0.40
7:G:28:ASP:HA	7:G:29:PRO:HD3	1.87	0.40
10:J:113:VAL:HG11	10:J:132:LEU:HD21	2.02	0.40
1:A:147:PHE:HD2	1:A:147:PHE:HA	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:65:ILE:HA	7:G:66:PRO:HD3	1.93	0.40
10:J:89:VAL:HG22	10:J:112:ILE:HB	2.03	0.40
3:C:54:ILE:HG22	3:C:80:LEU:HD13	2.03	0.40
10:J:696:LEU:HD21	10:J:813:MET:HG3	2.02	0.40
1:A:140:PHE:HB3	1:A:147:PHE:CZ	2.56	0.40
4:D:30:VAL:HG11	4:D:120:LEU:HD23	2.04	0.40
4:D:54:PRO:HB3	4:D:63:GLU:OE2	2.22	0.40
4:D:168:VAL:HG23	4:D:173:VAL:HB	2.03	0.40
6:F:101:LEU:O	6:F:104:LYS:NZ	2.54	0.40
9:I:17:ILE:HD11	9:I:58:ALA:HB2	2.02	0.40
10:J:293:PRO:CD	13:J:1101:BR:BR	3.24	0.40
11:K:576:LEU:HB2	11:K:577:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	298/304 (98%)	288 (97%)	10 (3%)	0	100	100
2	B	240/248 (97%)	235 (98%)	4 (2%)	1 (0%)	34	66
3	C	333/393 (85%)	313 (94%)	20 (6%)	0	100	100
4	D	221/245 (90%)	215 (97%)	5 (2%)	1 (0%)	29	61
5	E	265/267 (99%)	249 (94%)	16 (6%)	0	100	100
6	F	207/250 (83%)	192 (93%)	15 (7%)	0	100	100
7	G	234/242 (97%)	227 (97%)	7 (3%)	0	100	100
8	H	289/361 (80%)	281 (97%)	7 (2%)	1 (0%)	41	72
9	I	222/301 (74%)	216 (97%)	6 (3%)	0	100	100
10	J	942/1003 (94%)	901 (96%)	40 (4%)	1 (0%)	51	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	K	77/179 (43%)	71 (92%)	6 (8%)	0	100 100
All	All	3328/3793 (88%)	3188 (96%)	136 (4%)	4 (0%)	51 81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	167	ASP
4	D	140	LYS
8	H	121	ASN
10	J	598	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	253/265 (96%)	251 (99%)	2 (1%)	81 94
2	B	210/219 (96%)	209 (100%)	1 (0%)	88 96
3	C	290/349 (83%)	285 (98%)	5 (2%)	60 87
4	D	196/216 (91%)	196 (100%)	0	100 100
5	E	236/241 (98%)	235 (100%)	1 (0%)	91 97
6	F	182/219 (83%)	181 (100%)	1 (0%)	88 96
7	G	198/210 (94%)	195 (98%)	3 (2%)	65 89
8	H	242/313 (77%)	239 (99%)	3 (1%)	71 92
9	I	177/249 (71%)	175 (99%)	2 (1%)	73 92
10	J	812/901 (90%)	801 (99%)	11 (1%)	67 90
11	K	69/163 (42%)	69 (100%)	0	100 100
All	All	2865/3345 (86%)	2836 (99%)	29 (1%)	76 93

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	147	PHE
2	B	110	LYS
3	C	160	LEU
3	C	255	LEU
3	C	261	THR
3	C	384	ARG
3	C	391	ARG
5	E	122	PHE
6	F	201	VAL
7	G	4	PHE
7	G	137	PHE
7	G	158	VAL
8	H	119	VAL
8	H	126	VAL
8	H	318	ARG
9	I	49	ASN
9	I	286	ARG
10	J	72	LEU
10	J	80	SER
10	J	181	TYR
10	J	486	LEU
10	J	552	ASP
10	J	583	LEU
10	J	624	PHE
10	J	658	GLN
10	J	834	LEU
10	J	851	ASP
10	J	963	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	86	GLN
6	F	55	ASN
6	F	70	GLN
9	I	49	ASN
10	J	171	ASN
10	J	315	GLN
11	K	541	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	R	28/45 (62%)	9 (32%)	0

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	R	-39	A
12	R	-37	A
12	R	-33	G
12	R	-31	U
12	R	-14	U
12	R	-13	U
12	R	-12	U
12	R	-10	U
12	R	-6	U

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	GOL	H	404	-	5,5,5	0.37	0	5,5,5	0.30	0
14	GOL	H	402	-	5,5,5	0.38	0	5,5,5	0.26	0
14	GOL	G	301	-	5,5,5	0.37	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	GOL	H	403	-	5,5,5	0.37	0	5,5,5	0.34	0
15	MES	G	302	-	12,12,12	2.31	1 (8%)	15,16,16	1.95	5 (33%)
14	GOL	C	401	-	5,5,5	0.37	0	5,5,5	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	GOL	H	404	-	-	2/4/4/4	-
14	GOL	H	402	-	-	2/4/4/4	-
14	GOL	G	301	-	-	2/4/4/4	-
14	GOL	H	403	-	-	2/4/4/4	-
15	MES	G	302	-	-	0/6/14/14	0/1/1/1
14	GOL	C	401	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	302	MES	C8-S	-7.72	1.66	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	G	302	MES	C5-N4-C3	4.10	117.68	108.84
15	G	302	MES	C6-C5-N4	-3.08	105.44	110.12
15	G	302	MES	C7-N4-C5	2.24	117.20	111.24
15	G	302	MES	C7-N4-C3	2.07	116.74	111.24
15	G	302	MES	O1S-S-C8	2.00	109.75	106.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	G	301	GOL	O1-C1-C2-C3
14	H	402	GOL	O1-C1-C2-C3
14	H	403	GOL	O1-C1-C2-C3
14	H	404	GOL	O1-C1-C2-C3
14	G	301	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
14	C	401	GOL	O1-C1-C2-C3
14	H	404	GOL	O1-C1-C2-O2
14	C	401	GOL	O1-C1-C2-O2
14	H	402	GOL	O1-C1-C2-O2
14	H	403	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	402	GOL	1	0
14	H	403	GOL	1	0
15	G	302	MES	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	300/304 (98%)	-0.34	2 (0%)	87	84	31, 49, 110, 147	0
2	B	242/248 (97%)	-0.53	1 (0%)	92	91	29, 44, 88, 132	0
3	C	338/393 (86%)	-0.12	10 (2%)	50	40	35, 57, 127, 162	0
4	D	223/245 (91%)	-0.39	1 (0%)	92	91	32, 48, 76, 120	0
5	E	267/267 (100%)	-0.36	2 (0%)	87	84	35, 58, 106, 131	0
6	F	213/250 (85%)	-0.32	3 (1%)	75	70	36, 58, 115, 141	0
7	G	236/242 (97%)	-0.29	4 (1%)	70	63	32, 58, 122, 159	0
8	H	295/361 (81%)	-0.26	7 (2%)	59	49	38, 59, 114, 140	0
9	I	230/301 (76%)	0.10	15 (6%)	18	11	51, 80, 128, 140	0
10	J	948/1003 (94%)	-0.04	41 (4%)	35	25	47, 81, 136, 169	0
11	K	81/179 (45%)	0.16	6 (7%)	14	8	48, 90, 131, 143	0
12	R	30/45 (66%)	1.13	8 (26%)	0	0	72, 163, 201, 210	0
All	All	3403/3838 (88%)	-0.18	100 (2%)	51	41	29, 64, 128, 210	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	182	ASP	6.3
10	J	710	SER	6.1
5	E	265	LEU	6.0
9	I	1	MET	5.9
10	J	206	THR	5.9
11	K	532	ILE	5.6
8	H	276	SER	5.6
10	J	209	VAL	5.5
9	I	2	ALA	4.4
10	J	960	LEU	4.3
12	R	-39	A	4.2

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Mol	Chain	Res	Type	RSRZ
12	R	-37	A	4.1
12	R	-38	G	3.9
10	J	951	ALA	3.9
10	J	952	ALA	3.9
4	D	223	VAL	3.7
11	K	618	PHE	3.7
2	B	1	MET	3.6
10	J	941	LEU	3.6
10	J	210	GLU	3.4
9	I	162	PRO	3.4
10	J	973	VAL	3.4
3	C	258	THR	3.4
12	R	-44	C	3.3
10	J	205	ALA	3.3
3	C	265	SER	3.3
10	J	940	ARG	3.3
10	J	948	PRO	3.2
8	H	245	THR	3.2
9	I	185	ALA	3.2
10	J	970	PRO	3.1
10	J	958	TYR	3.1
11	K	537	ILE	3.1
3	C	253	SER	3.0
1	A	298	THR	3.0
10	J	711	ASP	3.0
10	J	961	THR	3.0
10	J	383	SER	3.0
10	J	211	SER	2.9
1	A	170	HIS	2.9
11	K	536	THR	2.9
12	R	-36	G	2.9
10	J	364	VAL	2.9
10	J	204	ALA	2.9
10	J	950	SER	2.8
3	C	9	THR	2.8
10	J	709	THR	2.8
11	K	534	LEU	2.8
9	I	70	LYS	2.8
8	H	275	GLU	2.8
7	G	51	GLY	2.7
10	J	949	ASN	2.7
10	J	942	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
9	I	66	CYS	2.6
10	J	924	ASN	2.6
7	G	1	MET	2.6
9	I	69	GLU	2.5
10	J	707	SER	2.5
10	J	1001	LYS	2.5
6	F	149	ASN	2.5
6	F	42	SER	2.5
8	H	50	SER	2.5
7	G	109	ASN	2.5
10	J	708	GLU	2.4
9	I	101	ARG	2.4
10	J	963	VAL	2.4
3	C	10	ILE	2.4
10	J	944	LEU	2.4
12	R	-43	C	2.4
10	J	281	SER	2.3
10	J	659	LEU	2.3
3	C	180	ASN	2.3
9	I	131	ASN	2.3
12	R	-40	G	2.3
8	H	51	ASP	2.3
8	H	240	ASP	2.3
9	I	67	GLU	2.3
9	I	49	ASN	2.3
3	C	181	GLU	2.2
10	J	956	VAL	2.2
5	E	163	ASP	2.2
9	I	5	PHE	2.2
9	I	106	ILE	2.2
8	H	357	ASN	2.2
3	C	179	ALA	2.2
12	R	-35	G	2.1
11	K	619	GLU	2.1
10	J	946	GLU	2.1
3	C	184	THR	2.1
10	J	925	GLY	2.1
7	G	2	SER	2.0
6	F	248	GLN	2.0
9	I	50	GLY	2.0
10	J	974	TYR	2.0
9	I	8	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
10	J	926	ILE	2.0
10	J	445	LEU	2.0
10	J	706	ASP	2.0
10	J	414	PRO	2.0
10	J	923	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	BR	J	1104	1/1	0.73	0.29	137,137,137,137	0
13	BR	A	402	1/1	0.82	0.25	136,136,136,136	0
14	GOL	H	403	6/6	0.87	0.24	72,74,77,81	0
14	GOL	G	301	6/6	0.89	0.19	81,85,91,92	0
14	GOL	H	402	6/6	0.92	0.22	66,72,77,77	0
16	MG	J	1105	1/1	0.92	0.11	72,72,72,72	0
15	MES	G	302	12/12	0.93	0.26	77,107,110,111	0
13	BR	I	301	1/1	0.93	0.07	90,90,90,90	0
14	GOL	C	401	6/6	0.94	0.17	79,83,84,84	0
13	BR	H	401	1/1	0.94	0.08	75,75,75,75	0
13	BR	J	1103	1/1	0.95	0.10	110,110,110,110	0
14	GOL	H	404	6/6	0.95	0.23	58,64,66,67	0
13	BR	E	301	1/1	0.96	0.09	101,101,101,101	0
13	BR	A	401	1/1	0.96	0.08	94,94,94,94	0
13	BR	J	1102	1/1	0.97	0.11	106,106,106,106	0
13	BR	J	1101	1/1	0.98	0.08	76,76,76,76	0
17	ZN	J	1106	1/1	0.98	0.13	62,62,62,62	0
13	BR	F	301	1/1	0.99	0.05	119,119,119,119	0

6.5 Other polymers (i)

There are no such residues in this entry.